

***In situ* XRD Studies of Phase Transitions in Lithiated Intermetallic Anodes**

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Intermetallic insertion compounds, to be used as anodes in lithium-ion batteries, have recently attracted much attention as alternatives to graphite, which is today the most commonly used anode material in commercial lithium-ion batteries. There is always a demand for new materials with higher energy densities, specific capacities and inherently better safety. Lithium alloys such as Li_xAl , Li_xSi and Li_xSn have been found to give both larger specific and volumetric capacities than graphite, but have so far not found practical use because of the large volume expansion and contraction that occurs during lithiation and delithiation.

Several intermetallic systems have shown an ability to insert lithium in a MM' host structure, in which M and M' are different metal atoms, to yield a $\text{Li}_x\text{MM}'$ product. This insertion reaction results in smaller volume changes during lithiation/delithiation than found for lithium-alloys. One example of such a system is copper-tin, Cu_6Sn_5 , with a NiAs-type structure into which Li ions can be inserted to yield a Li_2CuSn -type product with a lithiated zinc-blende-type structure [1]. The realisation that the CuSn zinc-blende framework of Li_2CuSn provides a three-dimensional interstitial space for lithium led to the investigation of intermetallic compounds with the zinc-blende structure, such as InSb [2]. The next step - to investigate transition-metal antimonides, especially copper antimonide, Cu_2Sb (Fig. 1) - was motivated by cost advantages and the relatively low reactivity of Cu. Also any extruded copper would be compatible with the copper current collector used for the negative electrode of lithium-ion cells [3]. On lithiation, a Li_2CuSb -type phase was formed, isostructural with the Li_2CuSn phase (Fig. 2). Complete lithitation resulted in full copper extrusion and the formation of Li_3Sb .

Emphasis is placed here on the structural transformations occurring during lithiation/delithiation as probed by *in situ* X-ray diffraction. The reaction mechanisms are set in relation to electrode performance.

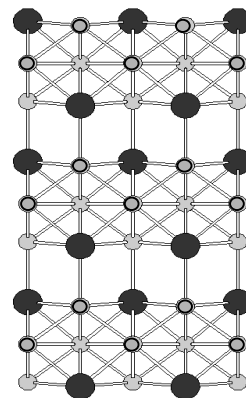


Fig. 1: The Cu_2Sb -structure (space group P4/nmm).

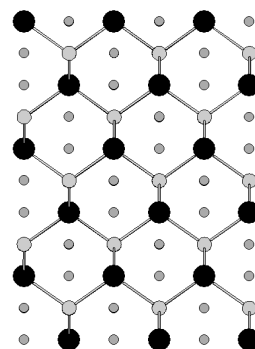


Fig. 2: A (001) projection of the Li_2CuSb -structure (space group F-43m).

References

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